Rotating Bose-Einstein condensates: Closing the gap between exact and mean-field solutions

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(Dated: January 23, 2015)

When a Bose-Einstein condensed cloud of atoms is given some angular momentum, it forms vortices arranged in structures with a discrete rotational symmetry. For these vortex states, the Hilbert space of the exact solution separates into a "primary" space related to the mean-field Gross-Pitaevskii solution and a "complementary" space including the corrections beyond mean-field. Considering a weakly-interacting Bose-Einstein condensate of harmonically-trapped atoms, we demonstrate how this separation can be used to close the conceptual gap between exact solutions for systems with only a few atoms and the thermodynamic limit for which the mean-field is the correct leading-order approximation. Although we illustrate this approach for the case of weak interactions, it is expected to be more generally valid.

PACS numbers: 03.75.Lm, 05.30.Jp, 67.85.Hj, 67.85.Jk

I. INTRODUCTION

Cold atomic quantum gases are typically dilute with an average interatomic distance much larger than the scattering length for atom-atom elastic collisions. This justifies the use of the mean-field approximation, which assumes a simple product form for the many-body wavefunction in the case of bosonic atoms. The complicated many-body problem is then reduced to one of a single variable, and the effect of interactions is described by a nonlinear term. This procedure was developed by Gross and Pitaevskii some decades ago [1, 2]. Since the experimental realization of Bose-Einstein condensation (BEC) in trapped atomic gases, this approach has been used with remarkable success, see e.g., Refs. [3–6].

One of the many fascinating effects associated with the superfluid properties of these gases is the formation of vortices in response to rotation. When the ratio of angular momentum to particle number increases, the number of vortices in the cloud grows, and they group in structures with discrete rotational symmetries (as illustrated by the mean-field densities in Fig. 1 below). Such vortex states have been observed in a number of experiments, see for example, Refs. [7–14]. The literature on this topic is extensive, as summarized by the reviews [15–19]. For a dilute and harmonically-trapped Bose-Einstein condensate of atoms, the rotational properties have been thoroughly analyzed both within the Gross-Pitaevskii approximation as in Refs. [20–25], and beyond the mean-field approximation as in Refs. [17, 22, 26–44].

Going beyond the mean-field approximation one often applies the so-called configuration-interaction (CI) formalism. In this numerical approach, one typically uses the Fock states constructed from a given set of single-particle states as a basis for the expansion of the exact many-body wavefunction. Other approaches are often variational, such as quantum Monte-Carlo [45] or density functional techniques for correlated Bose gases [46]. The so-called coupled-cluster approach, originally formulated for nuclei [47, 48] and often applied to atomic and molecular systems of fermions [49, 50] has also been adapted to bosonic systems [51] and is based on a series expansion of excitation operators acting on the corresponding mean-field ground state configuration.

An important advantage of the full CI approach is that apart from an almost always inevitable truncation of the Hilbert space, no further assumptions are made regarding the functional form of the many-body wavefunction. The method fully accounts for the correlations between the particles and accurately describes the low-lying excitations. However, the dimension of the Hamiltonian matrix grows very rapidly with the number of particles. Thus, little is currently known about the intermediate regime between small and large systems, in which exact diagonalization becomes prohibitively difficult but the mean-field approach still suffers from significant finite-size corrections.

Here, we wish to shed new light on this problem, suggesting a procedure that offers direct insight into the question of how a finite-size system of bosonic particles approaches the thermodynamic limit in which the Gross-Pitaevskii approach is known to be exact [33, 52–54]. With increasing particle number, we find a power-law convergence of the exact ground state into the mean-field Gross-Pitaevskii solution. Our study thus provides a clear and general strategy for this problem and offers strong arguments for both its validity and practicality. Further, these arguments are not limited by either the particle number or by the strength of the interaction.

II. ROTATIONAL PROPERTIES WITHIN THE GROSS-PITAEVSKII APPROXIMATION

We begin by briefly reviewing some of the well-known results regarding the formation of vortices in a weakly-interacting dilute Bose-Einstein condensate. The criterion adopted here for the formation of vortices is their

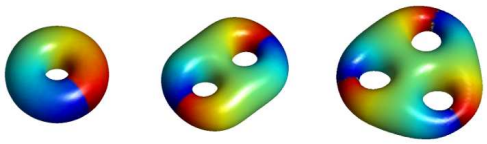

FIG. 1: Iso-surfaces of the density distribution of the bosonic cloud within the mean-field approximation (taken at about one third of the maximum value) for different ratios of angular momentum to particle number, $L/N = 1, 1.8$, and 2.3 from left to right (first discussed by Butts and Rokshar [20]). The vortices appear as holes, and the phase of the order parameter (in colorscale from red to blue) jumps by 2π when encircling each vortex.

energetic stability, namely the minimization of the energy either for a fixed value of the angular momentum or for a fixed value of the rotational frequency of the trap. We consider a harmonic trapping potential that is very tight along the axis of rotation, here chosen to be the z axis, with oscillator frequencies $\omega = \omega_x = \omega_y \ll \omega_z$. The two-body potential is assumed to be the usual contact interaction. For sufficiently weak interactions, $\hbar\omega_z$ is much larger than the interaction energy, and the atoms occupy only the ground state of the harmonic potential in the z-direction. Thus, the problem becomes effectively two-dimensional. The interatomic potential has the form $V(\mathbf{r}_i - \mathbf{r}_j) = u_0\,\delta(\mathbf{r}_i - \mathbf{r}_j)$, with $u_0 = U_0 \int |\phi(z)|^4\,dz$. Here $U_0 = 4\pi\hbar^2 a/M$ is the matrix element for elastic collisions, a is the corresponding scattering length, M is the mass of the particles, and $\phi(z)$ is the ground state of the oscillator potential along the z axis. The Hamiltonian that we consider is thus

$$\hat{H} = \sum_{i=1}^{N} -\frac{\hbar^2\nabla_i^2}{2M} + \frac{M}{2}\omega^2(x_i^2 + y_i^2) + \frac{u_0}{2}\sum_{i\neq j=1}^{N}\delta(\mathbf{r}_i - \mathbf{r}_j). \quad (1)$$

Within the mean-field Gross-Pitaevskii approximation the many-body wavefunction is assumed to have a product form, while the corresponding order parameter $\Psi_{\rm MF}(x, y)$ can be expanded in the eigenstates of the non-interacting problem. Making the assumption that the interaction energy is much smaller than $\hbar\omega$, it is sufficient to consider only the single-particle states $\phi_{0,m}$ of the lowest Landau level with zero radial nodes and angular momentum $m\hbar \geq 0$. (As we will explain in Sec. IV, the assumption of weak interactions is not essential, and the approach presented below is expected to remain valid for stronger interactions). The order parameter $\Psi_{\rm MF}$ is thus expanded in the basis of the states $\phi_{0,m}$, $\Psi_{\rm MF} = \sum_{m\geq 0} c_m\phi_{0,m}$, where the amplitudes c_m are variational parameters.

L/N	c_0	c_1	c_2	c_3	c_4	c_6
1.0	0	1.0000	0	0	0	0
1.8	0.4803	0	0.7992	0	-0.3611	-0.0127
2.3	0.5312	0	0	0.8179	0	-0.2210

TABLE I: Coefficients c_m of the expansion of the Gross-Pitaevskii order parameter in the lowest Landau level for $0 \leq m \leq 6$ (see text).

Minimizing the energy functional subject to the constraint of fixed L/N (where $L\hbar$ is the total angular momentum, and N the number of particles in the trap), one finds that as L/N increases, there is a sequence of phase transitions associated with the formation of one or more vortices in the gas (see the work by Butts and Rokshar [20] and, for example, Refs. [21–24, 41]). This is a direct consequence of the fact that for a fixed value of L/N only certain single-particle states are occupied by a macroscopic number of atoms of $\mathcal{O}(N)$. For example, for $L/N = 1$ the mean-field approximation yields a solution in which the only occupied single-particle state is the one with $m = 1$ and there is a single vortex at the trap center (see Refs. [20, 22, 26–28]). A similar behavior is found at higher values of L/N [20, 22]. For example, for $L/N = 1.8$, only the single-particle states with $m = 0, 2, 4, \ldots$ are occupied and the order parameter has two-fold symmetry. Correspondingly, for $L/N = 2.3$, the mean-field state consists of single-particle orbitals with only $m = 0, 3, 6, \ldots$ and it has three-fold symmetry. [56]

The actual values of the variational parameters c_m which are derived within this method are given in the Table below for $L/N = 1.0, 1.8$ and 2.3 (with $0 \leq m \leq 6$). In Fig. 1 we show the density isosurfaces for these states (having one-fold, two-fold, and three-fold symmetry), where the color scale (from red to blue) indicates that the phase of the order parameter changes by 2π when encircling the vortex singularity [20].

III. EXACT SOLUTIONS COMPARED TO MEAN-FIELD

In order to obtain the exact solution of the problem [26, 28, 33], one diagonalizes the many-body Hamiltonian $\hat{H}$ subject to the constraints of fixed particle number, $\sum_m n_m = N$, and fixed total angular momentum, $\sum_m mn_m = L$. With increasing values of N and L, the exponentially growing computational complexity severely restricts the size of numerically tractable systems to a few dozen atoms at most. Yet, studying the detailed structure of the exact wavefunction suggests a substantial simplification: In analogy with the mean-field approach discussed above, when an yrast state (i.e., the state with lowest energy at fixed angular momentum L) has a given discrete rotational symmetry, only certain single-particle states are occupied by a macroscopic number of atoms of $\mathcal{O}(N)$. This permits a separation of the total Hilbert space into a "primary" subspace that includes only Fock states constructed exclusively from single-particle states which are macroscopically occupied within the mean-field approximation and a far larger "complementary" space that consists of all other Fock states involving single-particle orbitals outside the mean-field space [44]. The inclusion of this complementary space leads to corrections to the mean-field energy that are of higher order in $1/N$ relative to the contribution from the primary space

[33]. We shall show in the following that this fact can be exploited efficiently to bridge the gap between the few-body and thermodynamic limits.

A. The "unit vortex"

We begin with the relatively simple case of $L/N = 1$, where (as described above) within the mean-field approximation only the $m = 1$ orbital is occupied. As a result there is a single vortex located at the centre of the trap. The primary space thus consists of only one Fock state, with all atoms occupying the $m = 1$ orbital. The complementary space is spanned by all other Fock states that have a non-zero occupancy of any single-particle state with $m \neq 1$. If one works within a truncated space including only the orbitals with $m = 0, 1$ and 2, the yrast state $|\Psi_0\rangle$ is known analytically to leading order in N [22, 26],

$$|\Psi_0\rangle = \sum_k \frac{(-1)^k}{\sqrt{2}^{k+1}} |0^k, 1^{N-2k}, 2^k\rangle, \qquad (2)$$

where the ket on the right denotes the Fock state with single-particle states in the lowest Landau level with $m = 0, 1$ and 2, and corresponding occupancies noted by the exponents. Returning to the separation of the full Hilbert space which we described above, the primary space consists of the single state with $k = 0$, with a probability $1/2$, while all the other states with $k \neq 0$ constitute the complementary space, with a probability also equal to $1/2$. Note that the amplitudes in Eq. (2) decrease exponentially with k, i.e., with the occupancy of the states belonging to the complementary space. As we will see below, this is a more general feature that also appears for larger values of the angular momentum.

We now consider a more systematic analysis of the convergence of the exact solution as a function of a gradual increase of the contribution from the complementary space. In order to capture fully the finite-size corrections, we extend the truncated space used in Eq. (2) by including the states with $0 \leq m \leq 6$ which necessitates the use of numerical methods. We evaluate the many-body states for a fixed number of particles n_1 in the $m = 1$ state (which is the occupation of the primary space) with the remaining $(N - n_1)$ particles in the complementary space. A Hamiltonian matrix is constructed for each value of $(N - n_1)$, and the single eigenstate of lowest interaction energy is selected from each matrix. A truncated Hamiltonian is built and diagonalized in this new basis of lowest-energy states to obtain the approximate energy spectrum $E_{\rm A}^i$ and the corresponding eigenfunctions $|\Psi_{\rm A}^i\rangle$ (where the index $i = 0, 1, 2, \ldots$ labels the excited states), here for the example of $N = 100$ atoms.

Figure 2 shows the low-energy spectrum as evaluated within this scheme, as a function of the highest occupancy of the complementary space N_c (red circles). (The energy is given in units of $v_0 = u_0 \int |\phi_{00}|^4 \, d^2r$, where ϕ_{00} is the single-particle ground state of the two-dimensional harmonic oscillator). The right side of this graph also shows the energy spectrum evaluated within the usual full diagonalization of the many-body Hamiltonian (blue circles) with the same truncation, $0 \leq m \leq 6$.

We see that there is a rapid convergence of the approximate solution to the exact result. Low-lying excited states are also reproduced fairly well, with larger deviations being apparent only in the higher-energy section of the spectrum. The relative error between the eigenenergies as evaluated within our model and with full diagonalization (in the same subspace) decreases exponentially with N_c. Remarkably, our method reproduces the yrast state as well as the low-lying excited states with high accuracy. As shown in panel (a) of Fig. 3 for the yrast state ("Y") and the first non-trivial excited state "G" that is related to the Goldstone mode [55], relative errors as small as 10^{-7} to 10^{-10} are obtained for values of $N_c \approx N/2$. (The first excited state, labeled "CM", is a trivial center-of-mass excitation). Panel (b) of Fig. 3 shows a logarithmic plot of the deviation from unity overlap of the model yrast state and the exact yrast state, $1 - |\langle \Psi_{\rm A}^0 \,|\, \Psi_{\rm ex} \rangle|^2$, as a function of N_c. This plot clearly shows an exponential convergence with the number of particles in the complementary space. Finally, Fig. 3 (c) shows the size of the submatrices arising in our calculations. Note that all of these submatrices are dramatically smaller than that of the full CI matrix, which has a dimension of $189,509$ for the specific example considered here.

B. States of discrete rotational symmetry

While the above example of the unit vortex at $L/N = 1$ is instructive, it is special in the sense that within the mean-field approximation there is only *one* state that is macroscopically occupied. We therefore consider, without loss of generality, the ratio $L/N = 9/5$ where within the mean-field approximation *two* vortices have nucleated in the cloud.

In what follows below we show how our method is applied considering this case as an example. We start with some approximate and semi-analytic results, which demonstrate the use of our method. At the end of this section we present the full numerical results.

In order to simplify the discussion, we first truncate the space to the single-particle states with $0 \leq m \leq 4$. (It is straightforward to generalize the arguments presented below to larger spaces). For large N, there is a macroscopic occupancy of the single-particle states with $m = 0,\ 2$ and 4 in the primary space. In this limit, it is convenient to approximate the exact yrast state by the sum

$$|\Psi_0\rangle \;=\; \sum_k (-1)^k \psi_k |0^{n_0(k)}, 2^{n_2(k)}, 4^{n_4(k)}\rangle, \qquad (3)$$

where the occupancy of the orbitals with $m = 0, 2$ and 4 are $n_0(k)$, $n_2(k)$ and $n_4(k)$, respectively. Fixing the occupancy of one orbital, for example, $n_0(k) = k$, the constraints of fixed particle number and fixed total angular momentum determine the occupancy of the other

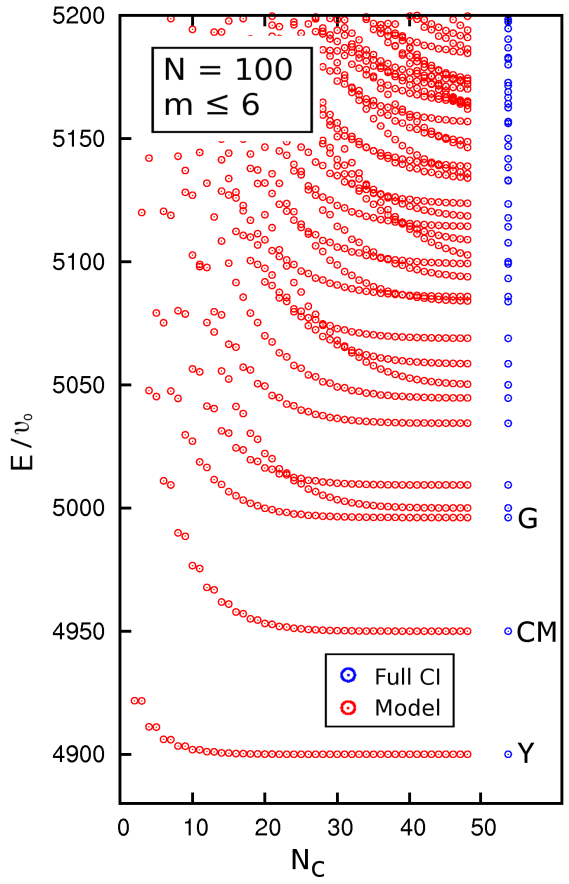

FIG. 2: Interaction energies (in units of v_0, see text) for $L = N = 100$ evaluated within the model (left, red circles) as a function of the highest occupancy N_c of the complementary space for a single-particle basis of orbitals with $0 \le m \le 6$. The blue bullets to the right show the result from the "exact" approach in the same subspace of single-particle states (see text). The relative error between the model and the full diagonalization in the same subspace is given in panel (b) of Fig. 3 for the yrast state ("Y") and the Goldstone mode ("G") (see text), converging to numbers as small as 10^{-7} to 10^{-10} for values of $N_c \approx N/2$. (The state labeled "CM" is a center-of-mass excitation).

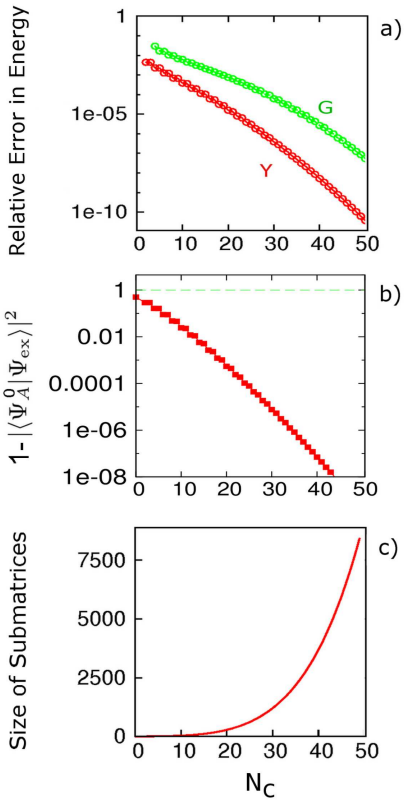

FIG. 3: (a) Relative error in the interaction energy, and (b) the deviation from unity overlap of the model yrast state with the exact yrast state, $1 - |\langle \Psi^0_{\rm A} | \Psi_{\rm ex} \rangle|^2$, on a logarithmic scale as a function of the highest occupancy of the complementary space, N_c, for the data of Fig. 2. Panel (c) shows the dimension of the submatrices as a function of N_c.

two. Consequently, for the above choice of $n_0(k)$, we have $n_2(k) = 11N/10 - 2k$ and $n_4(k) = k - N/10$. As discussed in Ref. [33], within the states contained in Eq. (3) the eigenvalue equation takes the form

$$-V_{k,k-1}\psi_{k-1} + V_{k,k}\psi_k - V_{k,k+1}\psi_{k+1} = E\psi_k. \qquad (4)$$

Here $V_{k,k'}$ are the matrix elements of the interaction V between the states $|k\rangle$ and $|k'\rangle$ on the right of Eq. (3), and E is the interaction energy. The above equation is obvious, since in addition to the diagonal matrix elements, the interaction, being a two-body operator, connects states where two atoms from the states with $m = 0$ and $m = 4$ get transferred to the state with $m = 2$, and vice versa.

Assuming that ψ_k is a smooth and differentiable function of k, this eigenvalue equation assumes the familiar form

$$-\frac{1}{2}(V_{k,k-1} + V_{k,k+1})\partial_k^2\psi_k + V_{\rm eff}(k)\psi_k = E\psi_k, \qquad (5)$$

where $V_{\rm eff}(k) = V_{k,k} - V_{k,k-1} - V_{k,k+1}$. In the vicinity of its minimum at some k_0 where $V_{\rm eff}$ has the value E_0, this effective potential can be approximated as $V_{\rm eff} - E_0 \propto (k-k_0)^2/2$. Thus, ψ_k satisfies an eigenvalue equation of a linear single-particle problem in the effective potential $V_{\rm eff}(k)$. For the example of $L/N = 9/5$, in the limit of very large N we find that the minimum of $V_{\rm eff}(k)$ occurs at $k_0/N = n_0/N \approx 0.2289$, a number that is very close to the value of the mean-field coefficient for $|c_0|^2 (\approx 0.2307)$ given in the Table above (albeit here for $0 \le m \le 4$). The energy of the yrast state within the primary space is found to be $E \approx (0.1880N^2 - 0.3149N)v_0$ plus terms of order unity. This expression for E must now be corrected at $\mathcal{O}(N)$ for the effects of the complementary space.

To gain insight into the role of the orbitals outside the mean-field space, we first consider contributions to the complementary space due to the $m = 1$ single-particle state only. The ψ_k in Eq. (3) for the yrast state is a Gaussian with a width of $\mathcal{O}(\sqrt{N})$. If one promotes $2n_1$ particles to the single-particle state with $m = 1$, where

n_1 is of $\mathcal{O}(N^0)$, to leading order in N, the corresponding yrast state can be written as

$$|2n_1\rangle \propto (a_1^\dagger a_1^\dagger a_0 a_2)^{n_1}|\Psi_0\rangle. \quad (6)$$

Here $|2n_1\rangle$ denotes the yrast state with $2n_1$ atoms in the single-particle state with $m = 1$ and $a_m^\dagger$ and a_m are the usual creation and annihilation operators for a particle with angular momentum $m\hbar$. The Gaussian form of the amplitudes of the primary space components of the state $|2n_1\rangle$ is preserved, and its center is simply shifted by a term of order unity. As before, the primary components are all of $\mathcal{O}(N)$ with a width of $\mathcal{O}(\sqrt{N})$, and the occupancy of the states in the complementary space is of $\mathcal{O}(N^0)$. As a consequence, the energy of the state $|2n_1\rangle$ is the same as that of $|\Psi_0\rangle$ to leading order in N, i.e., to $\mathcal{O}(N^2)$, and it is only necessary to consider corrections from the complementary space which are of subleading order, i.e., $\mathcal{O}(N)$. This implies that it is sufficient to approximate the full state of Eq. (3) by the single component $|\Psi_0\rangle = |0^{n_0(k_0)}, 2^{n_2(k_0)}, 4^{n_4(k_0)}\rangle$. This is a very considerable simplification.

Using this single component (appropriately renormalized to unity), we find that neither the curvature of $V_{\rm eff}$ nor the "inertial parameter" $(V_{k,k-1} + V_{k,k+1})$ depend on n_1 to leading order. Further, we find that the diagonal energies scale linearly with n_1, while the off-diagonal matrix elements $\langle 2n_1, 0|V|2n_1 + 2, 0\rangle$ are seen to be proportional to $N\sqrt{(2n_1 + 1)(2n_1 + 2)}$. These are the only nonzero off-diagonal matrix elements which come from the operator $a_1 a_1 a_0^\dagger a_2^\dagger$ (plus its Hermitian conjugate). Diagonalizing the resulting matrix, we find that the yrast energy becomes $E \approx (0.1880N^2 - 0.3885N)v_0$ and that the probabilities of the various states with $2n_1$ atoms in the $m = 1$ state decrease exponentially with n_1. We emphasize here that the above result is generic and not specific for the example that we have considered (see Appendix).

Let us now turn to the case where contributions from both the $m = 1$ and $m = 3$ single-particle orbitals are included in the complementary space. Generalizing Eq. (6), we see that the states including contributions from the complementary space can be constructed as

$$|2n_1 + 1, 2n_3 + 1\rangle \propto a_1^{\dagger 2n_1+1} a_3^{\dagger 2n_3+1} a_0^{n_1} a_2^{n_1+n_3+2} a_4^{n_3}|\Psi_0\rangle,$$

$$|2n_1, 2n_3\rangle \propto a_1^{\dagger 2n_1} a_3^{\dagger 2n_3} a_0^{n_1} a_2^{n_1+n_3} a_4^{n_3}|\Psi_0\rangle. \quad (7)$$

We emphasize that the counting of states in this equation is correct: Naively, one might expect that two distinct states, e.g., with $n_1 = n_3 = 1$ could be constructed from $|\Psi_0\rangle$ through the application of either $a_1^\dagger a_3^\dagger a_2 a_2$, or $a_1^\dagger a_3^\dagger a_0 a_4$. Given the Gaussian nature of ψ_k, however, these states are not orthogonal, and only one of them should be included.

There are four classes of nonzero off-diagonal matrix elements. The first two classes include

$$\langle n_1 + 2, n_3|\, V\, |n_1, n_3\rangle = \sqrt{n_0\, n_2} V_{11,20}\sqrt{(n_1 + 1)(n_1 + 2)},$$

and

$$\langle n_1, n_3 + 2|V|n_1, n_3\rangle = \sqrt{n_2\, n_4} V_{33,24}\sqrt{(n_3 + 1)(n_3 + 2)},$$

where $V_{ij,kl} = \langle \phi_{0i}, \phi_{0j}|V|\phi_{0k}, \phi_{0l}\rangle$. The remaining two classes reflect the staggering of the ground state wave function (i.e., the alternating sign seen explicitly in Eq. 2 above). They have the form

$$\langle n_1, n_3|V|n_1 - 1, n_3 + 1\rangle = (-1)^{n_3}\sqrt{n_1(n_3 + 1)} \times(2\sqrt{n_0\, n_2} V_{12,30} - 2\sqrt{n_2\, n_4} V_{14,30}) \quad (8)$$

and

$$\langle n_1 + 1, n_3 + 1|V|n_1, n_3\rangle = (-1)^{n_3}\sqrt{(n_1 + 1)(n_3 + 1)} \times(n_2 V_{22,13} - 2\sqrt{n_0\, n_4} V_{04,13}). \quad (9)$$

For N_c particles in the complementary space, the matrix has dimension $N_c/2 + 1$. Considering as an example $N_c = 18$, the yrast energy $E \approx (0.1880N^2 - 0.3149N)v_0$ obtained above for the primary space is shifted by the amount $\Delta E = -0.1893Nv_0$. As previously discussed for the simpler case with only the $m = 1$ orbital from the complementary space, the amplitudes show an exponential decrease with n_1 and n_3.

In the preceding paragraphs we approximated the yrast state with the single component $|\Psi_0\rangle = |0^{n_0(k_0)}, 2^{n_2(k_0)}, 4^{n_4(k_0)}\rangle$ which allowed us to give a detailed description of our method, providing us with some semi-analytic results. In what follows below we apply the same method fully numerically, without making the approximation for the yrast state consisting of a single component and compare it with the result of the full diagonalization (in the spirit of the case of $L/N = 1$ discussed above). Here, however, we consider only the yrast state, since the analysis of the excitation spectra beyond the value of $L/N = 1$ is more complicated due to the fact that, even for the low-lying states, competing solutions of different symmetry are found, see Ref. [44].

We follow the same procedure as above, considering two different truncations of the Hilbert space with $0 \le m \le 4$ and $0 \le m \le 6$. First, we evaluate the many-body states of Eq. (7) for each configuration of particles in the complementary space. Then, the lowest-energy state for each such configuration is chosen, and the truncated Hamiltonian is diagonalized in this new basis of lowest-energy states to obtain the approximate ground state energy E_A^0 and corresponding wavefunction $|\Psi_A^0\rangle$. Figure 4 shows the quantity $1 - |\langle\Psi_A^0|\Psi_{\rm ex}\rangle|^2$ versus N in the space $0 \le m \le 4$ (squares) and $0 \le m \le 6$ (circles), on a double-logarithmic scale. Intriguingly, for large N, this quantity shows a simple power-law behaviour, $1 - |\langle\Psi_A^0|\Psi_{\rm ex}\rangle|^2 \propto N^{-\gamma}$.

The fact that the overlap becomes worse for the more extended space, $0 \le m \le 6$, as compared to the more restricted one, $0 \le m \le 4$, is not a surprise, since the relative dimensionality of the full Hilbert space compared with the dimensionality of the space of our approach increases dramatically in the more extended space. The crucial result of this analysis is that the Fock state amplitudes for a given configuration in the complementary

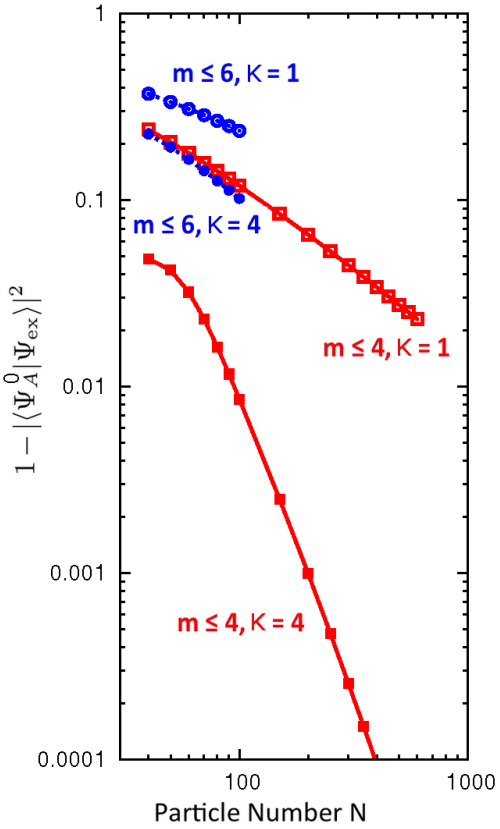

FIG. 4: The quantity $1-|\langle\Psi_A^0|\Psi_{\rm ex}\rangle|^2$ as a function of N for a fixed angular momentum per particle, $L/N=9/5$. Here, at each point the number N_c of particles in the complementary space was increased until numerical convergence of the result was obtained. The red squares refer to the space with $0\leq m\leq 4$ (open squares, $K=1$, and solid squares, $K=4$, where K is the number of lowest-energy states included in the reduced matrix), and the blue circles to the space with $0\leq m\leq 6$ (open circles, $K=1$, and solid circles, $K=4$).

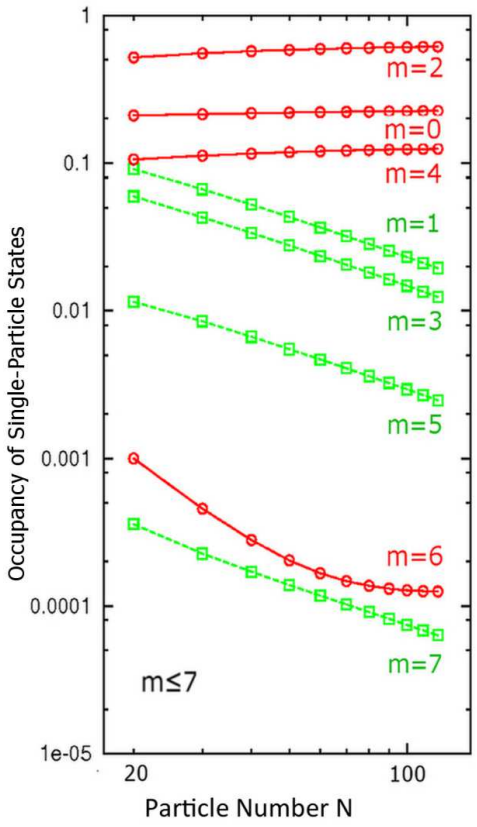

FIG. 5: Occupancies of the exact yrast states at $L/N=9/5$ as a function of the particle number, N, on a double-logarithmic scale here for a basis with $0\leq m\leq 7$. The saturation of the single-particle basis is reflected by the significant reduction in occupancy for higher values of m. The red circles indicate single-particle states that belong to the primary space; the green squares indicate those that belong to the complementary space. Clearly, with increasing N there is a convergence towards the occupancies obtained from mean-field (see the Table above).

space decrease exponentially with the number of particles in that space in both cases (we also emphasize that the number of the single-particle orbitals which are occupied by a macroscopic number of atoms saturates quickly for larger values of m, as it is clearly seen from the logarithmic plot of the occupancies in Fig. 5). The exponent is independent of N in the limit $N\to\infty$, indicating that the number of particles in the complementary space has a limit of $\mathcal{O}(N^0)$. This behavior is in fact strongly supported by the occupancies obtained through direct diagonalization, as seen also in Fig. 5. The occupancy of the states which construct the primary space in compliance with the mean-field approximation (red lines) increases (except for the orbital with $m=6$ that saturates), while the orbitals of the complementary states show a power-law decay with the number of particles.

More generally, one can retain the K eigenstates of lowest energy for each configuration of particles in the complementary space. (This corresponds to retaining excited states of the effective harmonic-oscillator problem in the primary space). For a given basis set, an increase of K accelerates the convergence towards the full solution (see Fig. 4). For fixed N, one finds exponential convergence in K. In this case, however, the exponent depends on N such that convergence is more rapid for larger particle numbers, and the generalized oscillator ground state *alone* contributes to the yrast state as $N\to\infty$. We stress that for $N_c=N$ and retaining all the possible K states, the approach is simply a passive unitary transformation of the basis and the results are necessarily identical to the full exact solution.

IV. CONCLUSIONS

In short, this paper suggests a significantly simplified understanding of the properties of a rotating Bose-Einstein condensate of trapped atoms. The direct numerical strategy for this problem would be to include a certain set of single-particle states and to diagonalize the resulting many-body Hamiltonian matrix. The difficulty is that the dimension of this matrix grows prohibitively

as the number of particles or the angular momentum (and thus, consequently, the number of necessary single-particle basis states) increases.

The method presented in this study makes use of the fact that only certain single-particle states are macroscopically occupied, while all other states have an occupancy of order unity. This introduces a natural separation of the Hilbert space into a primary and a complementary part. The first, containing the macroscopically occupied single-particle states, can be regarded as a generalised harmonic oscillator problem that can withstand major truncation when N is large. The resulting simplification is significant: The size of the Hamiltonian matrix can be reduced safely by a factor of order $N^{\kappa-2}$, where κ is the number of single-particle states included in the primary space. The contribution of the complementary subspace to the many-body states falls exponentially with the number of particles in it. Therefore, the present approach shows clearly that the vast majority of these states do not make a significant contribution to the yrast states, providing a simple understanding of how scattering processes between the primary and complementary spaces govern the transition from finite-sizes to the thermodynamic limit.

At mean-field level there are discontinuous phase transitions between states of different rotational symmetry corresponding to level crossings [44]. The states involved in such crossings can be constructed using the methods described here for distinct choices of the primary space. In the immediate vicinity of the crossing point, these states will be nearly degenerate and can in principle mix. Fortunately, however, the fact that they are based on different primary spaces ensures that matrix elements of the interaction between these states will vanish exponentially with the number of particles. Thus, such mixing becomes increasingly unimportant as the number of particles grows unless one is precisely at the crossing point.

The analysis presented here has been restricted to the limit of weak interactions, where one may neglect the single-particle eigenstates of the harmonic-oscillator potential with radial nodes. We stress, however, that our results are quite general and are *not* specific to this perturbative regime. Rather, the illustration of our method for the case of weak interactions represents a "proof of principle" and provides a representative example of our approach. Even in the regime of stronger interactions, which is actually of greater experimental relevance, one can solve the mean-field Gross-Pitaevskii equation to determine which states should be contained in our primary subspace. This subspace could, in principle, contain any or even all Landau levels with an angular momentum consistent with the discrete rotational symmetry of the ground state. In practice, mean-field calculations for stronger interactions show that the probability of finding states with n_r radial nodes in the mean-field wave function decreases exponentially with increasing n_r. The inclusion of additional Landau levels will not lead to any material complication in the construction or the solution of the generalized harmonic-oscillator problem described in Sec. III A. Excited Landau levels for other angular momenta will contribute to the complementary space. Since the exponential convergence found in the present manuscript is dictated by angular momentum considerations and not by the radial structure of the single-particle wave functions, this feature will be unaltered by the inclusion of higher Landau levels. In short, the scheme introduced here will remain valid and useful even if additional Landau levels are included. However, as mentioned above, internal convergence criteria must be adopted for assessing the accuracy of such calculations since full numerical diagonalizations will not be practical.

While the truncations adopted here appear to be particularly promising when the number of particles is large, we have not proven that the approach is a viable quantitative alternative to the exact diagonalization for large systems. Such a claim would require extensive benchmarking that is beyond the scope of this work and remains a matter for further investigation. Rather, the present study offers new and very explicit insight into the structure of the many-body wavefunction and its relation to the mean-field approximation for a rotating atomic superfluid. Although we have focused primarily on the yrast line, the procedure adopted here should also be suitable for investigating the richness of the excitation spectrum. We stress that the method is physically well-motivated and provides a well-defined transformation of the basis of many-body states that is completely passive in the sense that it suggests the order but not the degree of truncations of the basis.

Acknowledgments

We thank C. J. Pethick for discussions and helpful comments. This work was financially supported by the Swedish Research Council and the Nanometer Structure Consortium at Lund University, and the POLATOM ESF Research network.

APPENDIX: Toy Model

Consider, e.g., a real symmetric matrix which is zero except for the diagonal matrix elements $A_{n,n} = n-1$ and the off-diagonal matrix elements $A_{n,n\pm1}$, with $A_{n,n+1} = nf$. The eigenvalue equation

$$A_{n,n-1}c_{n-1} + A_{n,n}c_n + A_{n,n+1}c_{n+1} = Ec_n$$

has the form

$$(n-1)fc_{n-1} + (n-1)c_n + nfc_{n+1} = Ec_n.$$

The lowest eigenvalue of this matrix has a finite value in the limit that its dimension approaches infinity, provided that $0 \leq |f| \leq 1/2$. Subject to this restriction, the lowest eigenvalue is $E = -|f|x$ and the corresponding solution is $c_n = x^n\sqrt{1-x^2}$ with $x = -(1-\sqrt{1-4f^2})/(2f)$. For large values of n, the above eigenvalue equation has the simpler form $fc_{n-1} + c_n + fc_{n+1} = 0$, which has the

solution $c_n \propto x^n$, independent of E. In other words, c_n decays exponentially at precisely the same rate for all eigenvectors of finite energy. Although elementary, this toy model illustrates the present mechanism leading to exponential convergence.

[1] E. P. Gross, Nuovo Cimento **20**, 454 (1961).
[2] L. P. Pitaevskii, Zh. Eksp. Teor. Fiz. [Sov. Phys.-JETP **13**, 451 (1961)] **40**, 464 (1961).
[3] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999).
[4] A. J. Leggett, Rev. Mod. Phys. **73**, 307 (2001).
[5] C. J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases* (Cambridge University Press, 2002).
[6] L. P. Pitaevskii and S. Stringari, *Bose-Einstein Condensation* (Oxford Science Publications, 2003).
[7] F. Chevy, K. W. Madison, and J. Dalibard, Phys. Rev. Lett. **85**, 2223 (2000).
[8] K. W. Madison, F. Chevy, W. Wohlleben, and J. Dalibard, Phys. Rev. Lett. **84**, 806 (2000).
[9] K. W. Madison, F. Chevy, V. Bretin, and J. Dalibard, Phys. Rev. Lett. **86**, 4443 (2001).
[10] P. C. Haljan, I. Coddington, P. Engels, and E. A. Cornell, Phys. Rev. Lett. **87**, 210403 (2001).
[11] J. R. Abo-Shaer, C. Raman, J. M. Vogels, and W. Ketterle, Science **292**, 476 (2001).
[12] P. Engels, I. Coddington, P. C. Haljan, and E. A. Cornell, Phys. Rev. Lett. **89**, 100403 (2002).
[13] P. Engels, I. Coddington, P. C. Haljan, V. Schweikhard, and E. A. Cornell, Phys. Rev. Lett **90**, 170405 (2003).
[14] V. Schweikhard, I. Coddington, P. Engels, V. P. Mogendorff, and E. A. Cornell, Phys. Rev. Lett. **92**, 040404 (2004).
[15] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).
[16] S. Viefers, J. Phys. Cond. Mat. **20**, 123202 (2008).
[17] N. R. Cooper, Advances in Physics **57**, 539 (2008).
[18] A. L. Fetter, Rev. Mod. Phys. **81**, 647 (2009).
[19] H. Saarikoski, S. M. Reimann, A. Harju, and M. Manninen, Rev. Mod. Phys. **82**, 2785 (2010).
[20] D. A. Butts and D. S. Rokshar, Nature (London) **397**, 327 (1999).
[21] M. Linn and A. L. Fetter, Phys. Rev. A **60**, 4910 (1999).
[22] G. M. Kavoulakis, B. R. Mottelson, and C. J. Pethick, Phys. Rev. A **62**, 063605 (2000).
[23] M. Linn, M. Niemeyer, and A. L. Fetter, Phys. Rev. A **64**, 023602 (2001).
[24] J. J. García-Ripoll and V. M. Pérez-Garcia, Phys. Rev. A **63**, 041603(R) (2001).
[25] O. K. Vorov, P. V. Isacker, M. S. Hussein, and K. Bartschat, Phys. Rev. Lett. **95**, 230406 (2005).
[26] N. K. Wilkin, J. M. F. Gunn, and R. A. Smith, Phys. Rev. Lett. **80**, 2265 (1998).
[27] B. Mottelson, Phys. Rev. Lett. **83**, 2695 (1999).
[28] G. F. Bertsch and T. Papenbrock, Phys. Rev. Lett. **83**, 5412 (1999).
[29] A. D. Jackson and G. M. Kavoulakis, Phys. Rev. Lett. **85**, 2854 (2000).
[30] R. A. Smith and N. K. Wilkin, Phys. Rev. A **62**, 061602 (2000).
[31] T. Papenbrock and G. F. Bertsch, Phys. Rev. A **63**, 023616 (2001).
[32] W.-J. Huang, Phys. Rev. A **63**, 015602 (2001).
[33] A. D. Jackson, G. M. Kavoulakis, B. R. Mottelson, and S. M. Reimann, Phys. Rev. Lett. **86**, 945 (2001).
[34] X.-J. Liu, H. Hu, L. Chang, W. Zhang, S.-Q. Li, and Y.-Z. Wang, Phys. Rev. Lett. **87**, 030404 (2001).
[35] M. Manninen, S. M. Reimann, M. Koskinen, Y. Yu, and M. Toreblad, Phys. Rev. Lett. **94**, 106405 (2005).
[36] S. M. Reimann, M. Koskinen, Y. Yu, and M. Manninen, Phys. Rev. A **74**, 043603 (2006).
[37] S. M. Reimann, M. Koskinen, Y. Yu, and M. Manninen, New J. Phys. **8**, 59 (2006).
[38] M. I. Parke, N. K. Wilkin, J. M. F. Gunn, and A. Bourne, Phys. Rev. Lett. **101**, 110401 (2008).
[39] I. Romanovsky, C. Yannouleas, and U. Landman, Phys. Rev. A **78**, 011606 (2008).
[40] Z. Liu, H. Guo, S. Chen, and H. Fan, Phys. Rev. A **80**, 063606 (2009).
[41] D. Dagnino, N. Barberán, M. Lewenstein, and J. Dalibard, Nature Physics **5**, 431 (2009).
[42] D. Dagnino, N. Barberán, and M. Lewenstein, Phys. Rev. A **80**, 053611 (2009).
[43] T. Papenbrock, S. M. Reimann, and G. M. Kavoulakis, Phys. Rev. Lett. **108**, 075304 (2012).
[44] J. C. Cremon, G. M. Kavoulakis, B. R. Mottelson, and S. M. Reimann, Phys. Rev. A **87**, 053615 (2013).
[45] L. Pollet, Rep. Prog. Phys. **75**, 094501 ((2012)).
[46] F. Malet, P. Gori-Giorgi, et al., *work in preparation* (2014).
[47] F. Coester, Nucl. Phys. **7**, 421 (1958).
[48] F. Coester and H. Kümmel, Nucl. Phys. **17**, 477 (1960).
[49] R. J. Bartlett, J. Phys. Chem. **93**, 1697 (1989).
[50] R. F. Bishop, U. Kaldor, H. Kümmel, and D. Mukherjee, *The Coupled Cluster Approach to Quantum Many-Particle Systems* (Springer, Heidelberg, 2003).
[51] L. S. Cederbaum, O. E. Alon, and A. Streltsov, Phys. Rev. A **73**, 043609 (2006).
[52] E. H. Lieb, R. Seiringer, and J. Yngvason, Phys. Rev. A **61**, 043602 (2000).
[53] E. H. Lieb, R. Seiringer, and J. Yngvason, Phys. Rev. A **79**, 063626 (2009).
[54] M. Lewin and R. Seiringer, J. Stat. Phys. **137**, 1040 (2009).
[55] M. Ueda and T. Nakajima, Phys. Rev. A **73**, 043603 (2006).
[56] We note that generally there is a saturation in the necessary size of the basis with increasing single-particle angular momentum m. This is shown in Fig. 5 for the example of the two-vortex state, where the occupancy of orbitals with $m > 4$ is reduced by orders of magnitude.